

\* \* \* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \*  
d hist

(FILE 'HOME' ENTERED AT 10:32:14 ON 03 SEP 2002)

FILE 'REGISTRY' ENTERED AT 10:32:23 ON 03 SEP 2002

L1                   STRUCTURE UPLOADED  
L2        47 S L1  
L3        34 S L2 AND 1/NRRS  
L4        3 S L3 AND 1/CNRS  
L5                   STRUCTURE UPLOADED  
L6        7 S L5  
L7        2 S L6 AND 1/CNRS  
L8                   STRUCTURE UPLOADED  
L9        7 S L8  
L10      2 S L9 AND 1/CNRS  
L11                   STRUCTURE UPLOADED  
L12      5 S L11  
L13      0 S L12 AND 1/CNRS  
L14      834 S L11 FULL  
L15      219 S L14 AND 1/CNRS  
L16      219 S L14 AND 1/NRS  
L17      0 S L14 AND 1/NNRS  
L18      612 S L14 AND 1/NRRS  
L19      200 S L18 AND (8/SZ OR 9/SZ OR 10/SZ OR 11/SZ OR 12/SZ OR 13/SZ OR

FILE 'CAPLUS' ENTERED AT 11:52:08 ON 03 SEP 2002

L20     1 S L19 AND (BETA(W)TURN? OR GAMMA(W)TURN?)

FILE 'REGISTRY' ENTERED AT 11:53:14 ON 03 SEP 2002

FILE 'CAPLUS' ENTERED AT 11:53:17 ON 03 SEP 2002

L21     4 S L19 AND (COMBINATOR? OR LIBRAR?)  
          E "402955-03-7"/BI 25  
L22     1 S E3 OR E4  
          E "426219-04-7"/BI 25  
L23     1 S E3 OR E4  
L24     1 S L23  
          E "333435-69-1"/BI 25  
L25     1 S E3 OR E4

FILE 'REGISTRY' ENTERED AT 12:14:15 ON 03 SEP 2002

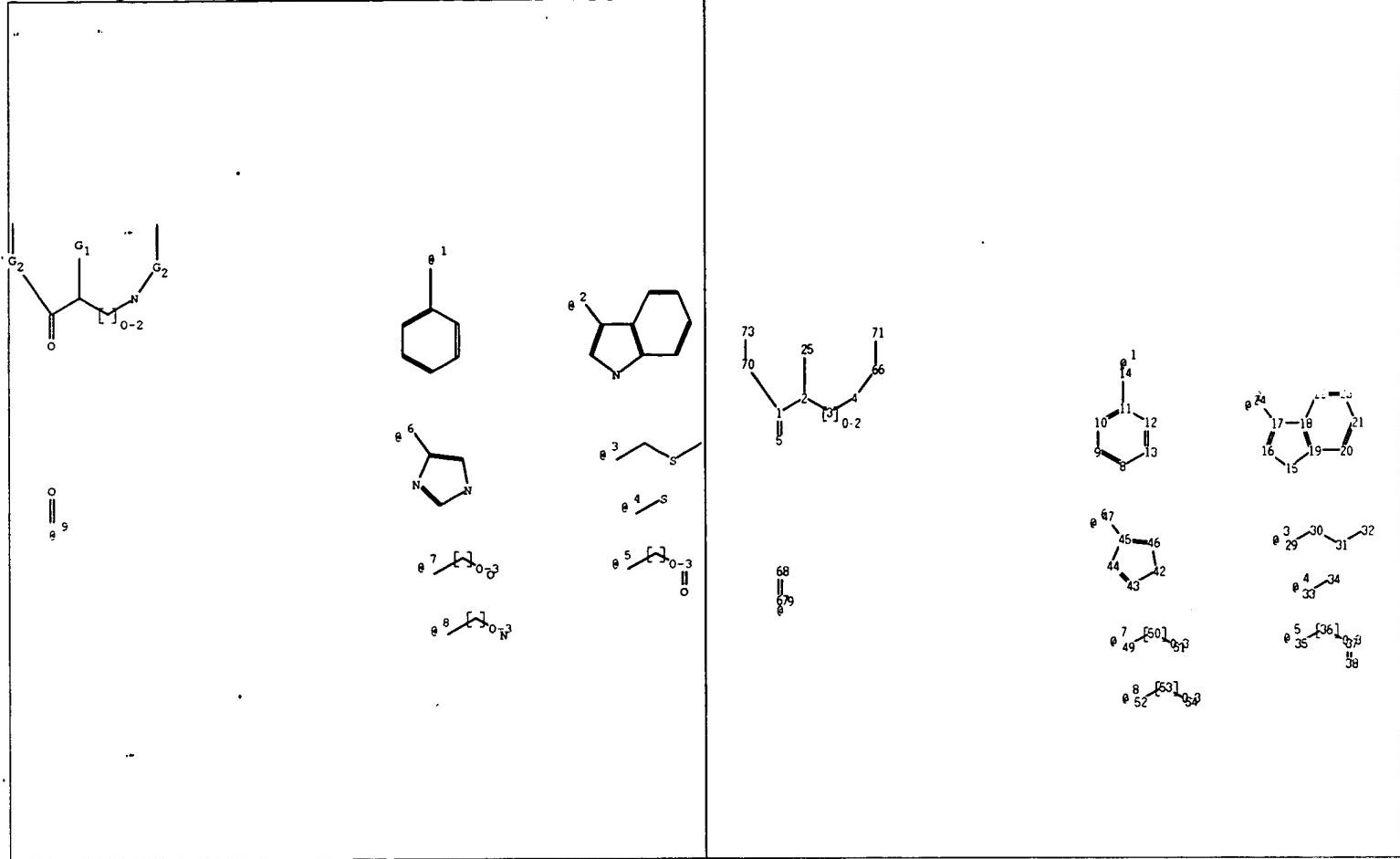
L26     1 S 333439-06-8/RN

FILE 'CAPLUS' ENTERED AT 12:30:20 ON 03 SEP 2002

L27     E "333439-06-8"/BI 25  
          1 S E3 OR E4

FILE 'MARPAT' ENTERED AT 12:31:10 ON 03 SEP 2002

SET NOTICE DISPLAY 1  
SET NOTICE LOGIN DISPLAY



chain nodes :

5 14 24 25 29 30 31 32 33 34 35 36 37 38 47 49 50 51 52  
53 54 67 68

ring nodes :

1 2 3 4 8 9 10 11 12 13 15 16 17 18 19 20 21 22 23 42  
43 44 45 46 66 70 71 73

chain bonds :

1-5    2-25    11-14    17-24    29-30    30-31    31-32    33-34    35-36    36-37    37-38  
45-47    49-50    50-51    52-53    53-54    67-68

ring bonds :

1-2 1-70, 2-3 3-4 4-66 8-9 8-13 9-10 10-11 11-12 12-13 15-16  
15-19 16-17 17-18 18-19 18-22 19-20 20-21 21-23 22-23 42-43  
42-46 43-44 44-45 45-46 66-71 70-73

.exact/norm bonds :

1-5 1-2 1-70 2-3 3-4 4-66 15-16 15-19 16-17 17-18 30-31 31-32  
33-34 37-38 42-43 42-46 43-44 44-45 45-46 50-51 53-54 66-71  
67-68 70-73

exact bonds :

**2-25    11-14    17-24    29-30    35-36    36-37    45-47    49-50    52-53**

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13 18-19 18-22 19-20 20-21 21-23  
22-23

G1: H, CH<sub>3</sub>, Et, n-Pr, i-Pr, i-Bu, s-Bu, [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7], [\*8]

G2 : CH<sub>2</sub>, NH, O, [\*9]

Hydrogen count :

```
2:= exact 1 3:= exact 2 71:>= minimum 2 73:>= minimum 2
Match level :
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom
 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 29:CLASS
 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
 37:CLASS 38:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:CLASS
 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 66:CLASS
 67:CLASS 68:CLASS 70:CLASS 71:CLASS 73:CLASS
```